Lyapunov Exponents, Transport and the Extensivity of Dimensional Loss

Kenichiro Aoki[a] and Dimitri Kusnezov[b]
[a] *Dept. of Physics, Keio University, 4—1—1 Hiyoshi, Kouhoku–ku, Yokohama 223–8521, Japan*
[b] *Center for Theoretical Physics, Sloane Physics Lab, Yale University, New Haven, CT 06520-8120*

An explicit relation between the dimensional loss (ΔD), entropy production and transport is established under thermal gradients, relating the microscopic and macroscopic behaviors of the system. The extensivity of ΔD in systems with bulk behavior follows from the relation. The maximum Lyapunov exponents in thermal equilibrium and ΔD in non-equilibrium depend on the choice of heat-baths, while their product is unique and macroscopic. Finite size corrections are also computed and all results are verified numerically.

Fractal structures in phase space have become the focus of attention in the understanding of the relationship between microscopic dynamics and macroscopic non-equilibrium physics [1]. In the escape-rate formalism, the properties of a fractal repellor are known to govern the transport [2]. In contrast, in boundary driven non-equilibrium steady states, the stationary distribution is generally fractal, but the precise connection to transport is not fully understood [1]. This reduction in dimension, ΔD, has been argued to be related to transport [3–5], although the only precise understanding arises in the weak field limit of the Lorentz gas [3], which does not have clear generalization to non-equilibrium many-body systems. The presence of fractals has also been used to demonstrate how the second law of thermodynamics is consistent with time-reversal invariant, deterministic dynamics [6]. Many of these issues require the understanding of the Lyapunov spectrum, whose analytic properties are known only in certain special cases [7]. In this letter we study general Hamiltonians coupled to two heat baths at different temperatures at opposite sides of the system, generating heat flow. We will see that the type of heat baths chosen affect ΔD and the Lyapunov exponents, for the same boundary temperatures. We investigate the meaning and the origins of extensivity of ΔD in systems with bulk behavior, including finite size corrections, and relate them to transport. The new relations are verified numerically. We systematically study the system not only close to but also far from equilibrium, as well as the dependence on the heat-baths themselves. While the extensivity of dimensional loss has been disputed due to the incompatibility with local equilibrium [3], we will see that this is not an issue.

In systems with bulk behavior, to say that ΔD behaves "extensively" means that ΔD should remain relatively the same under the same local non-equilibrium conditions when we change the size of the system. For systems in thermal gradients, one might expect

$$\frac{\Delta D}{D}=C'\left(\frac{\nabla T}{T}\right)^2+\mathcal{O}\left(\left(\frac{\nabla T}{T}\right)^4\right) \tag{1}$$

where the constant C' might depend on T. Such a behavior is particularly natural if one envisions that a continuum limit of the theory ultimately exists. ΔD has been studied previously for color conduction [8,9,3], sheared fluids [10,4,5] and thermal conduction [4], numerically. Analytic computations of the Lyapunov spectrum and ΔD have understandably been restricted to small or idealized systems such as the Lorentz gas [11,3,7]. The physical properties are far from trivial; even whether ΔD generally arises has been an issue [12]. Extensivity of ΔD under thermal gradients has been analyzed [4], but the relation to transport and entropy production was not elucidated previously. Extensivity has been investigated in sheared fluids [9,5] and for color conductivity [8,9]. Study of the dependence on the number and types of thermostats or systematic analysis far from equilibrium have not been performed before.

We first discuss the properties of ΔD, its extensivity and its relation to transport. Consider a system with cross-sectional area A placed in contact with two heat-baths at both ends having temperatures (T_1^0, T_2^0). The Lyapunov spectrum $\{\lambda_j\}_{j=1,2,\ldots,D}$ distills the microscopic properties of the classical system and are the time averaged eigenvalues of the stability matrix $(\partial\dot{\varphi}_i/\partial\varphi_j)$, where $\{\varphi_j\}_{j=1,2,\ldots,D}$ are all the degrees of the freedom of the system, *including* the heat-baths. From the spectrum, we may compute the fractal dimension using the Kaplan–Yorke estimate D_{KY}, which has the property that $\Delta D\equiv D-D_{KY}>0$ in non-equilibrium and $\Delta D=0$ in equilibrium systems. While the extensivity relation (1) is natural, the relation is ill-defined for two reasons: First, ∇T is in general *not* constant within the system and which ∇T we choose visibly affects the results [13]. Second, it is unclear what D in the denominator should mean. It can be the number of degrees of freedom of the whole system including the thermostats, that without, or that only of the interior. These difficulties arise since D_{KY} is a global quantity defined only for the whole system. An expression consistent with (1) in the near equilibrium limit that suffers no such ambiguity even far from equilibrium is (denoting the heat flux by J),

$$\frac{\Delta D}{V_{in}} = C_D J^2 \tag{2}$$

since J is constant throughout the system. V_{in} is the interior volume of the system. We shall derive this relation near equilibrium and further verify it numerically.

Computing ΔD requires the full Lyapunov spectrum, which involves evolving $D^2 + D$ degrees of freedom. This apparently makes it difficult to explicitly check extensivity. Close to equilibrium, this difficulty can be overcome as follows [8,5]. Define $\Delta D_{max}, \Delta D_{min}$ as

$$\Delta D_{max} \equiv -\frac{\sum_{j=1}^{D} \lambda_j}{\lambda_{max}}, \qquad \Delta D_{min} \equiv \frac{\sum_{j=1}^{D} \lambda_j}{\lambda_{min}} \tag{3}$$

where $\lambda_{max}, \lambda_{min}$ are the maximum and minimum exponents. When $\Delta D \leq 1$, $\Delta D_{min} = \Delta D$ holds *exactly.* (More generally, when $K - 1 < \Delta D \leq K$, we need only to compute $\sum_{j=1}^{D} \lambda_j$ and the K lowest Lyapunov exponents to obtain ΔD.) This holds when the system is close to equilibrium. $\nabla T/T \sim 1/L$ and $\Delta D \sim L^{d-2}$ (in d-dimensions) so that ΔD is always small for large systems in 1-d. Since $\lambda_{min} = -\lambda_{max}$ in equilibrium, ΔD_{max} should also be a good approximation to ΔD, close to equilibrium. We analyze these conditions systematically in the following and make these conditions more precise. $\sum_{j=1}^{D} \lambda_j$, the total rate of phase space contraction, can be computed from the equations of motion of $\{\varphi_j\}$ alone and λ_{max} can be computed from evolving one tangent vector, so we need only to evolve $2D$ degrees of freedom to compute ΔD_{max} — a huge reduction for large D.

We now systematically investigate how the extensivity of ΔD arises. First note that $\sum_{j=1}^{D} \lambda_j$ is the rate of entropy production, $\dot{S}$, for the system [1,8]. We use this to derive a thermodynamic relation [13]

$$\begin{aligned}\sum_{j=1}^{D} \lambda_j &= -\dot{S} = AJ\left(\frac{1}{T_1^0} - \frac{1}{T_2^0}\right) \\ &= \frac{V_{in} J^2}{\kappa T^2}\left(1 + \frac{2\alpha\kappa}{V_{in}}\right) + \mathcal{O}(J^4)\end{aligned} \tag{4}$$

where κ is the thermal conductivity. We have included the effects of boundary temperature jumps that behave as αJ when the jumps are not too big [14]. α, which arises as a finite size correction, measures the efficacy of the heat-baths, which can be stochastic or deterministic, and can have significant effects as will be shown. Notice that (4) always holds, both close to and far from equilibrium and is independent of the type and number of thermostats used. Further, it is V_{in} that arises in the relation, rather than D.

λ_{max} behaves as $\lambda_{max} = \lambda_{max}^{eq} + \mathcal{O}(J^2)$, where λ_{max}^{eq} is its equilibrium value. λ_{max}^{eq} is *independent* of V_{in} for large enough systems, but can depend on T and also on the thermostats used. Close to equilibrium, the above behavior of $\sum_{j=1}^{D} \lambda_j$ and λ_{max}^{eq}, when combined, explain the extensivity of ΔD as in (2). In this limit, the extensivity of ΔD arises from $\sum_{j=1}^{D} \lambda_j$ and the thermostat dependence from λ_{max}^{eq}. Since C_D can be derived in the $J \to 0$ limit, we derive

$$C_D = \frac{1}{\kappa \lambda_{max}^{eq} T^2}\left(1 + \frac{2\alpha\kappa}{V_{in}}\right) \overset{V_{in} \to \infty}{\longrightarrow} \frac{1}{\kappa \lambda_{max}^{eq} T^2} \tag{5}$$

which relates macroscopic transport and entropy production to the microscopic ΔD. A subtlety needs to be mentioned: We have found that λ_{max}^{eq} is consistent with having a finite large volume limit but have not proven this statement analytically. In fact, this difficult issue is open and there have been conflicting results on the existence of the thermodynamic limit of λ_{max}^{eq} [15]. From our argument, we see that the extensive nature of ΔD requires that λ_{max}^{eq} have a thermodynamic limit or vice versa. We note that in systems without a bulk limit, such as the FPU model, ΔD needs not be extensive and λ_{max}^{eq} needs not have a thermodynamic limit, which might explain some of the discrepancy seen in the previous literature [15]. Far from equilibrium, ΔD and ΔD_{max} will be quite different, yet the extensivity relation (2) can and seems to still hold for ΔD. This reflects the deeper geometric significance of ΔD not present in ΔD_{max}.

While the above theory is valid in any dimension, we now apply it to the 1–d ϕ^4 theory described by the following Hamiltonian:

$$H = \sum_{x=1}^{L}\left[\frac{\pi_x^2}{2} + \frac{(\nabla\phi_x)^2}{2} + \frac{\phi_x^4}{4}\right] \quad . \tag{6}$$

We choose the ϕ^4 theory because it is a classic statistical model that naturally appears in broad physical contexts. Also, the statistical properties of the theory have been studied previously, including thermal transport which has bulk behavior [13,16]. We model the heat-baths dynamically by applying Nosé-Hoover (NH) thermostats or their variants (demons) at the boundaries, as explained in [13]. The interior includes the dynamics only of the ϕ^4 theory. Temperature is defined unambiguously using the ideal gas thermometer, $T(x) = \langle \pi_x^2 \rangle$. The number of (heat-bath) boundary sites thermostatted on each end, N_B, will be varied. We employ one set of thermostats per thermostatted site. We run the simulations with time steps of 10^{-3} to 0.05 for 10^6 to 10^9 steps, understanding its convergence properties and also checking that the results do not change with the step size. To obtain the Lyapunov spectrum, we use the method in [17,8].

Let us first look at the dependence of ΔD, ΔD_{max} and ΔD_{min} with respect to J (Fig. 1). We see that close enough to equilibrium, all three quantities agree and display J^2 behavior as in (2) and (5). Remarkably, even far from equilibrium and well into the non–linear regime, ΔD has a robust J^2 behavior, but not $\Delta D_{max,min}$. We further note that the boundary temperature jumps have a significant effect, the effect being larger for smaller T. For instance, using $\kappa = 2.83(4)T^{-1.35(2)}$, $\alpha = 2.6(1)$ [13], $2\alpha\kappa = 300, 6$ for $T = 0.1, 2$, respectively.

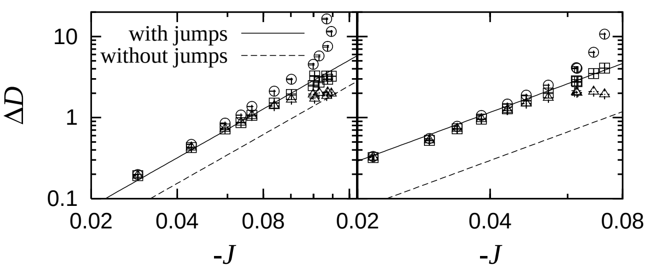

FIG. 1. ΔD ($\Box$), ΔD_{max} ($\circ$) and ΔD_{min} ($\triangle$) against $-J$ in $L = 11$ (left), $L = 41$ (right) at $T = 0.5$ for the $N_B = 1$ case. J^2 behavior with and without finite size corrections are also shown. ΔD displays J^2 behavior even for large $-J$.

Performing an analysis similar to those performed for Fig. 1, we can extract the proportionality constant $\Delta D/J^2$ for a particular L, N_B and T. Combining this data for various $V_{in}(= L - 2N_B + 1)$, N_B, we find that the relations (2),(5) describe the results quite well over a few orders in magnitude (Fig. 2). We have also included the data of [4] which used *stochastic* thermostats and see that the formulas work quite well.

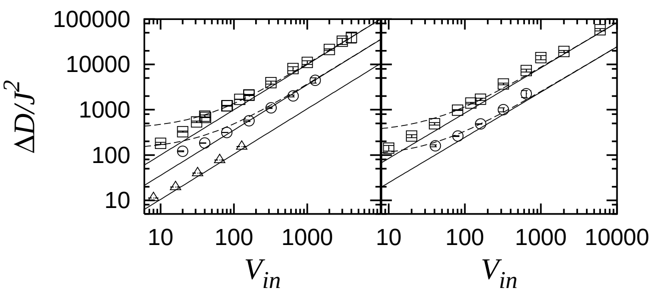

FIG. 2. (left) $\Delta D/J^2$ against V_{in} for $N_B = 1$ ($\Box$), $N_B = 40$ ($\circ$), with NH thermostats (left) and demons (right) at $T = 0.5$. $V_{in}/(\kappa\lambda_{max}^{eq}T^2)$ (solid) and $V_{in}/(\kappa\lambda_{max}^{eq}T^2)(1 + 2\alpha\kappa/V_{in})$ (dashes) are plotted. Application of the formulas to the data of [4] ($\triangle$) works very well (data and formulas rescaled by 5000 for plotting).

There are a few subtleties which we now resolve: First, we can and have made the distinction between the total volume and V_{in} in the formula (2), since we have performed analyses with $N_B = 1 \sim 40$ sites. Secondly, C_D can and does depend on T and also on the type of thermostats used, including N_B. C_D has similar behavior both for NH thermostats and for demons, with the former being larger, and both decreasing with N_B. Since the demons have twice the number of degrees of freedom per thermostatted site compared to NH thermostats, this is quite remarkable. Furthermore, somewhat surprisingly, when we increase N_B by one, thereby *increasing* the total number of degrees of freedom by 6(8) in the NH thermostat (demons) case, C_D *decreases* and so does ΔD for the same J. The reason for this will be clarified below.

We study examples of the behavior of $\sum_{j=1}^{D} \lambda_j$ in Fig. 3 (left). We see that the entropy production relation Eq. (4) works well near and far from equilibrium, and that the quadratic behavior with respect to J can be observed close to equilibrium. This is true, *independently* of the type of thermostats used. On the other hand, λ_{max}^{eq} can and does

depend on the type of thermostats used as well as T (Fig. 3 (right)). This is responsible for the thermostat dependence of C_D seen in Fig. 2. The larger λ^{eq}_{max} for demons and the increase seen with N_B are quite natural since the existence of more thermostats lead to more chaotic behavior.

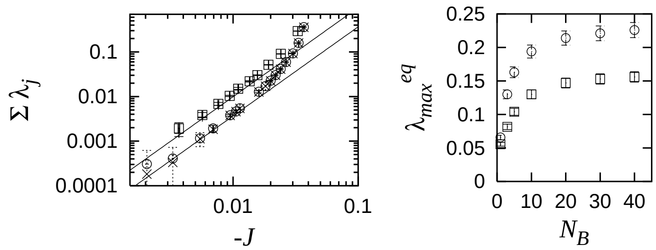

FIG. 3. (left) $\sum_{j=1}^{D}\lambda_j$ and $J\left(1/T_1^0 - 1/T_2^0\right)$ with respect to $-J$, for $T = 0.5$ ($\square, +$), $T = 2$ ($\circ, \times$) and their quadratic behavior Eq. (4) near equilibrium (solid) for the $L = 162$, $N_B = 1$ case. The quantities agree excellently.
(right) The dependence of the λ^{eq}_{max} on N_B at $T = 0.5$ for NH thermostats ($\square$) and demons ($\circ$). This demonstrates that λ^{eq}_{max} is strongly heat-bath dependent, and is not uniquely determined by the local equilibrium conditions.

We now study in detail the difference between ΔD, ΔD_{min} and ΔD_{max}: Let us first work out what the condition $\Delta D \leq 1$ means. Define $r \equiv \Delta T/T$, where T is the central temperature and ΔT is the difference in the boundary temperatures so that $r \leq 2$, always, and $\nabla T \simeq rT/V_{in}$. Then, we can derive a simple estimate,

$$\Delta D \leq 1 \quad \Leftrightarrow \quad V_{in} \geq \frac{\kappa\left(\nabla T\right)^2}{\lambda^{eq}_{max} T^2} \simeq r^2 \frac{\kappa}{\lambda^{eq}_{max}} \tag{7}$$

Let us analyze $T = 0.5$ case more concretely; the condition is most stringent for $N_B = 1$ (NH) case, when λ^{eq}_{max} is the smallest. So we obtain the condition $V_{in}/r^2 \gtrsim 130$ for $\Delta D \leq 1$ and for large lattices, $V_{in} \gtrsim 400$, it should be satisfied for any gradient, which is consistent with our results. While we did not consider here the non-linearity of the profiles, the boundaries temperature jumps and the non-linearity of the response [14,18], we are in some sense close to equilibrium when $\Delta D \leq 1$ so that the rough arguments suffice for the purpose at hand.

When $\Delta D \leq 1$, how large is the difference $\Delta D_{max} - \Delta D$? In this case, $\Delta D_{min} = \Delta D$, as explained above, so we need to consider $\lambda_{max} + \lambda_{min}$, which is zero in equilibrium since the Lyapunov spectrum is symmetric with respect to sign inversion [1]. As we move away from equilibrium, the behavior can be described by $\lambda_{max}/\lambda_{min} + 1 = C_\lambda J^2 + \mathcal{O}\left(J^4\right)$. Then, when $\Delta D \leq 1$,

$$\frac{\Delta D_{max} - \Delta D}{\Delta D} \simeq C_\lambda J^2 \leq \frac{C_\lambda}{V_{in} C_D} \tag{8}$$

For $N_B = 1$, $T = 0.5$, $C_\lambda = 13L^{0.5}$, so that $(\Delta D_{max} - \Delta D)/\Delta D \lesssim 0.1 \times (V_{in}/100)^{-0.5}$. Since the statistical errors are typically at a few % level, the difference between ΔD and ΔD_{max} is at most comparable to them except for small systems, when $\Delta D \leq 1$. In Fig. 1, it can indeed be seen that for $\Delta D \leq 1$, ΔD_{max} agrees with ΔD within error. Similar analysis can be applied at different T.

When $\Delta D \geq 1$, the relation $\Delta D_{min} = \Delta D$ no longer holds exactly and the deviations from it is of $\mathcal{O}(\delta\lambda/\lambda)$, with $\delta\lambda$ being the sum of the differences of the exponents λ_j ($j > D_{KY}$), which is *not* zero even in equilibrium. $\delta\lambda/\lambda \sim \Delta D/D$ so that in systems with small relative dimensional loss, ΔD_{max} can still be a good approximation. In Fig. 1, we see that when $\Delta D \gtrsim 1$, ΔD_{max} is in general not a good approximation to ΔD and that it is a clearly better approximation there for the larger system.

We derived the extensivity of ΔD in systems with bulk behavior under thermal gradients in (2), thereby making the notion precise. The extensivity was explicitly related to the macroscopic transport properties as in (5) through entropy production. Previously, it was emphasized that the extensivity of ΔD is not compatible with local equilibrium so that it is questionable [3]. It is now known that systems such as ϕ^4 theory in $d = 1 - 3$ display violations of local equilibrium under thermal gradients in a similar manner, as $\sim \left(\nabla T/T\right)^2$ [18]. This resolves the apparent conflict since the violations of local equilibrium emerge in a manner analogous to (2).

We further explicitly verified that ΔD in ϕ^4 theory behaves extensively under various thermal gradients for $L \lesssim 10^4$ and its relation to transport. The relations (2),(4) and (5), however, are more general. We saw that the relations applied well to [4] which used *stochastic* thermostats in a different model. An application to dilute gas using the standard estimates of λ_{max} [1] yields $C_D \simeq 2/[\rho v^2 \ln(4l/d)]$, where ρ is the density, v is the average particle velocity, l is the mean free path and d is the particle diameter. Then for $\nabla T/T \sim 0.01\,\mathrm{m}^{-1}$, $\Delta D \sim 10^8\,\mathrm{m}^{-3}$ at room temperature — quite large, yet far smaller than the total number of degrees of freedom.

We find the results satisfying from the physics point of view: Since ΔD pertains to the whole system, it includes the temperature profile which is curved in general, boundary temperature jumps and the various types of thermostats. Yet, ΔD can be related to macroscopic transport with the thermostat dependence cleanly separated into λ_{max}. Furthermore, ΔD has extensive behavior with respect to the internal volume wherein the system is manifestly in non-equilibrium. We have seen that λ^{eq}_{max} is *not* unique: In global thermal equilibrium, different choices of heat-baths can lead to very different values. The result is that dimensional loss is not unique either, only the product $\Delta D \lambda^{eq}_{max}$ behaves macroscopically and can be related to thermodynamic quantities.

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